



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2017 – 11:54 pm GMT

PDB ID : 4GLM  
Title : Crystal structure of the SH3 Domain of DNMBP protein [Homo sapiens]  
Authors : Dong, A.; Guan, X.; Huang, H.; Tempel, W.; Gu, J.; Sidhu, S.; Bountra, C.;  
Arrowsmith, C.H.; Edwards, A.M.; Tong, Y.; Structural Genomics Consortium  
(SGC)  
Deposited on : 2012-08-14  
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

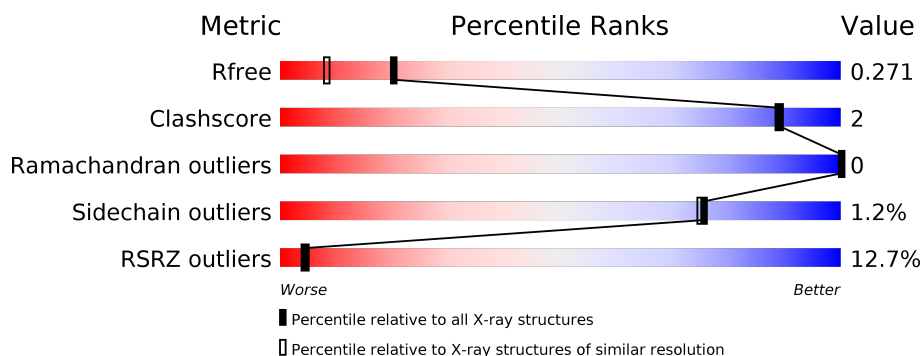
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	72	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>79%</span> <span>19%</span> </div> </div>
1	B	72	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>76%</span> <span>21%</span> </div> </div>
1	C	72	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">24%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>72%</span> <span>6%</span> <span>22%</span> </div> </div>
1	D	72	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">15%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>76%</span> <span>21%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	B	402	-	-	-	X
2	UNX	B	405	-	-	-	X
2	UNX	B	406	-	-	-	X
2	UNX	C	401	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1981 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dynamin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	58	Total	C	N	O	S	0	2	1
			465	305	78	81	1			
1	B	57	Total	C	N	O	S	0	6	0
			482	320	76	85	1			
1	C	56	Total	C	N	O	S	0	3	0
			441	289	71	80	1			
1	D	57	Total	C	N	O	S	0	0	0
			436	289	66	80	1			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	GLY	-	EXPRESSION TAG	UNP Q6XZF7
A	234	GLY	-	EXPRESSION TAG	UNP Q6XZF7
A	235	ALA	-	EXPRESSION TAG	UNP Q6XZF7
A	236	ALA	-	EXPRESSION TAG	UNP Q6XZF7
A	237	GLN	-	EXPRESSION TAG	UNP Q6XZF7
A	238	PRO	-	EXPRESSION TAG	UNP Q6XZF7
A	239	ALA	-	EXPRESSION TAG	UNP Q6XZF7
A	240	MET	-	EXPRESSION TAG	UNP Q6XZF7
A	241	ALA	-	EXPRESSION TAG	UNP Q6XZF7
A	242	GLN	-	EXPRESSION TAG	UNP Q6XZF7
A	243	GLY	-	EXPRESSION TAG	UNP Q6XZF7
A	244	ALA	-	EXPRESSION TAG	UNP Q6XZF7
A	245	LEU	-	EXPRESSION TAG	UNP Q6XZF7
A	302	ALA	-	EXPRESSION TAG	UNP Q6XZF7
A	303	ALA	-	EXPRESSION TAG	UNP Q6XZF7
A	304	ALA	-	EXPRESSION TAG	UNP Q6XZF7
B	233	GLY	-	EXPRESSION TAG	UNP Q6XZF7
B	234	GLY	-	EXPRESSION TAG	UNP Q6XZF7
B	235	ALA	-	EXPRESSION TAG	UNP Q6XZF7
B	236	ALA	-	EXPRESSION TAG	UNP Q6XZF7
B	237	GLN	-	EXPRESSION TAG	UNP Q6XZF7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	238	PRO	-	EXPRESSION TAG	UNP Q6XZF7
B	239	ALA	-	EXPRESSION TAG	UNP Q6XZF7
B	240	MET	-	EXPRESSION TAG	UNP Q6XZF7
B	241	ALA	-	EXPRESSION TAG	UNP Q6XZF7
B	242	GLN	-	EXPRESSION TAG	UNP Q6XZF7
B	243	GLY	-	EXPRESSION TAG	UNP Q6XZF7
B	244	ALA	-	EXPRESSION TAG	UNP Q6XZF7
B	245	LEU	-	EXPRESSION TAG	UNP Q6XZF7
B	302	ALA	-	EXPRESSION TAG	UNP Q6XZF7
B	303	ALA	-	EXPRESSION TAG	UNP Q6XZF7
B	304	ALA	-	EXPRESSION TAG	UNP Q6XZF7
C	233	GLY	-	EXPRESSION TAG	UNP Q6XZF7
C	234	GLY	-	EXPRESSION TAG	UNP Q6XZF7
C	235	ALA	-	EXPRESSION TAG	UNP Q6XZF7
C	236	ALA	-	EXPRESSION TAG	UNP Q6XZF7
C	237	GLN	-	EXPRESSION TAG	UNP Q6XZF7
C	238	PRO	-	EXPRESSION TAG	UNP Q6XZF7
C	239	ALA	-	EXPRESSION TAG	UNP Q6XZF7
C	240	MET	-	EXPRESSION TAG	UNP Q6XZF7
C	241	ALA	-	EXPRESSION TAG	UNP Q6XZF7
C	242	GLN	-	EXPRESSION TAG	UNP Q6XZF7
C	243	GLY	-	EXPRESSION TAG	UNP Q6XZF7
C	244	ALA	-	EXPRESSION TAG	UNP Q6XZF7
C	245	LEU	-	EXPRESSION TAG	UNP Q6XZF7
C	302	ALA	-	EXPRESSION TAG	UNP Q6XZF7
C	303	ALA	-	EXPRESSION TAG	UNP Q6XZF7
C	304	ALA	-	EXPRESSION TAG	UNP Q6XZF7
D	233	GLY	-	EXPRESSION TAG	UNP Q6XZF7
D	234	GLY	-	EXPRESSION TAG	UNP Q6XZF7
D	235	ALA	-	EXPRESSION TAG	UNP Q6XZF7
D	236	ALA	-	EXPRESSION TAG	UNP Q6XZF7
D	237	GLN	-	EXPRESSION TAG	UNP Q6XZF7
D	238	PRO	-	EXPRESSION TAG	UNP Q6XZF7
D	239	ALA	-	EXPRESSION TAG	UNP Q6XZF7
D	240	MET	-	EXPRESSION TAG	UNP Q6XZF7
D	241	ALA	-	EXPRESSION TAG	UNP Q6XZF7
D	242	GLN	-	EXPRESSION TAG	UNP Q6XZF7
D	243	GLY	-	EXPRESSION TAG	UNP Q6XZF7
D	244	ALA	-	EXPRESSION TAG	UNP Q6XZF7
D	245	LEU	-	EXPRESSION TAG	UNP Q6XZF7
D	302	ALA	-	EXPRESSION TAG	UNP Q6XZF7
D	303	ALA	-	EXPRESSION TAG	UNP Q6XZF7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	304	ALA	-	EXPRESSION TAG	UNP Q6XZF7

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	6	Total X 6 6	0	0
2	A	8	Total X 8 8	0	0
2	D	1	Total X 1 1	0	0
2	C	3	Total X 3 3	0	0

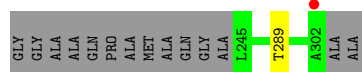
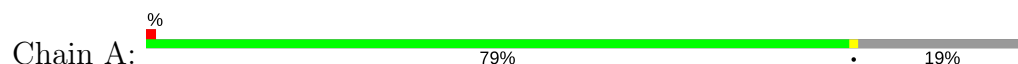
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	43	Total O 44 44	0	1
3	B	53	Total O 54 54	0	1
3	C	14	Total O 15 15	0	1
3	D	25	Total O 26 26	0	1

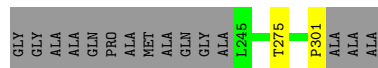
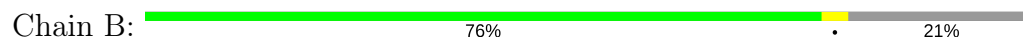
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Dynamamin-binding protein



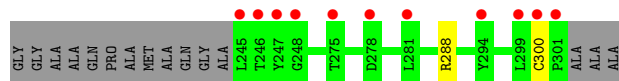
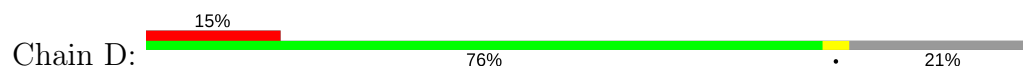
#### • Molecule 1: Dynamamin-binding protein



#### • Molecule 1: Dynamamin-binding protein



#### • Molecule 1: Dynamamin-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.28Å 136.20Å 33.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.82 – 1.90 35.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.82-1.90) 99.9 (35.82-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 1.91Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.229 , 0.259 0.233 , 0.271	Depositor DCC
$R_{free}$ test set	915 reflections (4.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.35 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2049e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.56	0/482	0.58	0/653
1	B	0.55	0/511	0.60	0/692
1	C	0.46	0/460	0.57	0/625
1	D	0.47	0/447	0.57	0/609
All	All	0.51	0/1900	0.58	0/2579

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	465	0	461	1	0
1	B	482	0	492	5	0
1	C	441	0	420	7	0
1	D	436	0	407	2	0
2	A	8	0	0	0	0
2	B	6	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	54	0	0	0	0
3	C	15	0	0	0	0
3	D	26	0	0	0	0
All	All	1981	0	1780	8	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 8 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:THR:HG21	1:C:275:THR:H	1.67	0.60
1:B:275:THR:CG2	1:C:275:THR:O	2.58	0.51
1:B:275:THR:HG21	1:C:275:THR:N	2.25	0.50
1:B:275:THR:HG21	1:C:275:THR:O	2.12	0.50
1:A:289[B]:THR:HG23	3:A:1124:HOH:O	2.15	0.47

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	58/72 (81%)	58 (100%)	0	0	100	100
1	B	61/72 (85%)	61 (100%)	0	0	100	100
1	C	57/72 (79%)	57 (100%)	0	0	100	100
1	D	55/72 (76%)	55 (100%)	0	0	100	100
All	All	231/288 (80%)	231 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	47/52 (90%)	47 (100%)	0	100	100
1	B	51/52 (98%)	51 (100%)	0	100	100
1	C	43/52 (83%)	41 (95%)	2 (5%)	30	19
1	D	41/52 (79%)	40 (98%)	1 (2%)	54	47
All	All	182/208 (88%)	179 (98%)	3 (2%)	75	65

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	253[A]	ARG
1	C	253[B]	ARG
1	D	300	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	58/72 (80%)	0.31	1 (1%) 70 73	16, 25, 48, 62	0
1	B	57/72 (79%)	0.23	0 100 100	15, 25, 46, 58	0
1	C	56/72 (77%)	1.62	17 (30%) 0 0	38, 54, 75, 110	0
1	D	57/72 (79%)	1.21	11 (19%) 1 1	31, 51, 81, 117	0
All	All	228/288 (79%)	0.84	29 (12%) 4 4	15, 39, 73, 117	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	PRO	8.9
1	D	301	PRO	8.2
1	C	300	CYS	6.8
1	C	299	LEU	6.5
1	D	294	TYR	5.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	UNX	B	405	1/1	0.85	0.45	21.42	30,30,30,30	0
2	UNX	C	401	1/1	0.86	0.38	6.20	30,30,30,30	0
2	UNX	B	402	1/1	0.77	0.30	5.32	30,30,30,30	0
2	UNX	B	406	1/1	0.96	0.29	5.10	30,30,30,30	0
2	UNX	B	403	1/1	0.87	0.16	1.13	30,30,30,30	0
2	UNX	C	403	1/1	0.82	0.17	1.01	30,30,30,30	0
2	UNX	A	1001	1/1	0.70	0.18	0.26	30,30,30,30	0
2	UNX	A	1002	1/1	0.75	0.22	-	30,30,30,30	0
2	UNX	A	1004	1/1	0.78	0.13	-	30,30,30,30	0
2	UNX	B	404	1/1	0.83	0.24	-	30,30,30,30	0
2	UNX	A	1006	1/1	0.89	0.09	-	30,30,30,30	0
2	UNX	A	1008	1/1	0.93	0.22	-	30,30,30,30	0
2	UNX	B	401	1/1	0.52	0.23	-	30,30,30,30	0
2	UNX	D	401	1/1	0.88	0.09	-	30,30,30,30	0
2	UNX	A	1005	1/1	0.78	0.32	-	30,30,30,30	0
2	UNX	A	1003	1/1	0.91	0.11	-	30,30,30,30	0
2	UNX	A	1007	1/1	0.88	0.35	-	30,30,30,30	0
2	UNX	C	402	1/1	0.82	0.16	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.